

# Fundamentals in generalized elasticity and dislocation theory of quasicrystals: Green tensor, dislocation key-formulas and dislocation loops

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## Abstract

The present work provides fundamental quantities in generalized elasticity and dislocation theory of quasicrystals. In a clear and straightforward manner, the three-dimensional Green tensor of generalized elasticity theory and the extended displacement vector for an arbitrary extended force are derived. Next, in the framework of dislocation theory of quasicrystals, the solutions of the field equations for the extended displacement vector and the extended elastic distortion tensor are given; that is the generalized Burgers equation for arbitrary sources and the generalized Mura-Willis formula, respectively. Moreover, important quantities of the theory of dislocations as the Eshelby stress tensor, Peach-Koehler force, stress function tensor and the interaction energy are derived for general dislocations. The application to dislocation loops gives rise to the generalized Burgers equation, where the displacement vector can be written as a sum of a line integral plus a purely geometric part. Finally, using the Green tensor, all other dislocation key-formulas for loops, known from the theory of anisotropic elasticity, like the Peach-Koehler stress formula, Mura-Willis equation, Volterra equation, stress function tensor and the interaction energy are derived for quasicrystals.

**Keywords:** quasicrystals; anisotropic elasticity; Green tensor; dislocations; Burgers formula; interaction energy

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# 1 Introduction

The knowledge of Green functions is of fundamental importance for many physical, mathematical and engineering problems. In the theory of partial differential equations, a Green function is the fundamental solution of a linear partial differential equation (see, e.g., [1]). Using the elastic Green tensor function, one can immediately calculate the displacement field caused by external forces in an infinite linear elastic medium. Lord Kelvin [2] found the three-dimensional solution for an isotropic elastic medium. Lifshitz and Rosenzweig [3] and Synge [4] (see also [5, 6]) derived the three-dimensional elastic Green tensor for arbitrary anisotropic materials.

Quasicrystals were discovered by Shechtman in 1982 (see Shechtman et al. [7]). Due to the discovery of quasicrystals, the International Union of Crystallography changed the official definition of a crystal in 1992. For a clarification on the important subject of the definition of a quasicrystal we refer to Lifshitz [8, 9]. Shechtman was awarded the 2011 Nobel Prize in Chemistry for his great discovery. Quasicrystals are materials possessing long-range order but no translational symmetry. Nowadays, quasicrystals represent an interesting class of novel materials. Their particular (physical, electronic, thermodynamical, chemical, etc.) properties attract more and more the attention of researchers from various fields and their application to several domains is highly increasing. For instance, Kenzari et al. [10] show that the use of quasicrystals in additive manufacturing technology has advantages compared to other composites used today, due to their reduced friction and improved wear resistance, offering an improved functional performance. Moreover, they show that the functional parts contain almost no porosity and are leak-tight allowing their direct use in many fluidic applications. A systematic and comprehensive overview of the field of quasicrystals covering various aspects of the theory of elasticity and defects (cracks, dislocations) is given by Fan [11].

Three-dimensional Green functions play an important role in the theory of elasticity and defects. They have not only pure mathematical merits themselves, but are also important in the performance of approximative methods (finite element method, boundary element method) as well as in the study of cracks, dislocations and inclusions. In the literature, only some special cases of Green functions are known for quasicrystals so far. De and Pelcovits [12] found the two-dimensional Green functions for pentagonal (2D) quasicrystals and Ding et al. [13] calculated the explicit expressions of two-dimensional Green tensors for various forms of planar (2D) quasicrystals. Bachteler and Trebin [14] gave an approximative solution for the three-dimensional Green tensor of icosahedral (3D) quasicrystals, assuming that the coupling between phonons and phasons is small (perturbation method).

In the present work, we start by deriving an analytical expression for *the three-dimensional elastic Green tensor for one-, two-, and three-dimensional quasicrystals* in analogy to the theory of anisotropic elasticity, using Fourier transform. Based on the three-dimensional Green tensor another important quantity, *the tensor of the potential of the second gradient of the Green tensor*, is also introduced for quasicrystals. The extended displacement vector for an arbitrary extended force in elasticity theory of quasicrystals is also given. The mathematical structure of the higher dimensionality of quasicrystals leads in a natural way to the introduction of *the hyperspace notation*,

which unifies the phonon and phason fields to the corresponding *extended field* in the hyperspace. Throughout the paper the hyperspace notation is used providing straightforward calculations.

The main part of this work is devoted to the study of dislocations in quasicrystals. We generalize all the key-formulas of dislocations known from the theory of anisotropic elasticity (e.g., [15, 16, 17]) towards quasicrystals. In particular, we deduce the generalized Burgers formula, Mura-Willis formula, Peach-Koehler stress formula, Peach-Koehler force, Eshelby stress tensor and the interaction energy for general dislocations, that means for discrete dislocations or a continuous distribution of dislocations. The generalized Burgers formula is derived following a straightforward method introduced by Lazar and Kirchner [17] which gives directly the decomposition of the displacement vector into a part depending on the solid angle, and a line integral part depending on the material constants. In addition, special focus is given on the derivation of the corresponding key-formulas for dislocation loops. Up to now, only solutions of straight dislocations have been found for quasicrystals (see, e.g., [11]). It should be emphasized that the extended elastic distortion and stress tensors as well as the extended displacement vector produced by a dislocation loop can be written in terms of derivatives of the three-dimensional Green tensor. In this way, the obtained dislocation key-equations build the basis of a field theory formulation of dislocations in quasicrystals.

The paper is organized as follows. In Section 2, the basic framework of the generalized elasticity theory of quasicrystals with emphasis to the introduction of the hyperspace notation is presented. The three-dimensional elastic Green tensor and the extended displacement vector for an arbitrary extended force are derived. Section 3 is devoted to the dislocation theory of quasicrystals. In subsections 3.1-3.5, we derive all the dislocation key-formulas, including the  $J$ -integral. Finally, subsection 3.6 provides the application to dislocation loops with the generalized Burgers equation and all other dislocation key-formulas for loops. Conclusions are given in Section 4. In the Appendices A and B, we give some details about the calculation of the three-dimensional Green tensor and its gradient.

## 2 Generalized elasticity theory of quasicrystals

### 2.1 Basic framework

This subsection is devoted to the basic framework of the generalized elasticity theory of quasicrystals with a special focus to the introduction of the hyperspace notation. It is a compact notation which facilitates significantly the calculations throughout the paper.

An  $(n - 3)$ -dimensional quasicrystal can be generated by the projection of an  $n$ -dimensional periodic structure to the 3-dimensional physical space ( $n = 4, 5, 6$ ). The  $n$ -dimensional hyperspace  $E^n$  can be decomposed into the direct sum of two orthogonal subspaces,

$$E^n = E_{\parallel}^3 \oplus E_{\perp}^{(n-3)}, \quad (1)$$

where  $E_{\parallel}^3$  is the 3-dimensional physical or parallel space of the phonon fields and  $E_{\perp}^{(n-3)}$  is the  $(n - 3)$ -dimensional perpendicular space of the phason fields. For  $n = 4, 5, 6$  we

speak of 1D, 2D, 3D quasicrystals and the dimension of the hyperspace is 4D, 5D, 6D, respectively. Throughout the text, phonon fields will be denoted by  $(\cdot)^\parallel$  and phason fields by  $(\cdot)^\perp$ . It is important to note that all quantities (phonon and phason fields) depend on the so-called material space coordinates  $\mathbf{x} \in \mathbb{R}^3$ .

In the theory of quasicrystals, the equilibrium conditions are of the form (see, e.g., [18, 19])

$$\sigma_{ij,j}^\parallel + f_i^\parallel = 0, \quad (2)$$

$$\sigma_{ij,j}^\perp + f_i^\perp = 0, \quad (3)$$

where  $\sigma_{ij}^\parallel$  and  $\sigma_{ij}^\perp$  are the *phonon and phason stress tensors*, respectively, and  $f_i^\parallel$  is the *conventional (phonon) body force density* and  $f_i^\perp$  is a *generalized (phason) body force density*. The comma denotes differentiation with respect to the material coordinates. We note that the phonon stress tensor is symmetric,  $\sigma_{ij}^\parallel = \sigma_{ji}^\parallel$ , while the phason stress tensor is asymmetric,  $\sigma_{ij}^\perp \neq \sigma_{ji}^\perp$  (see, e.g., [18]).

In the theory of compatible elasticity, the *phonon and phason distortion tensors*,  $\beta_{kl}^\parallel$  and  $\beta_{kl}^\perp$ , are defined as the spatial gradients of the *phonon and phason displacement vectors*,  $u_k^\parallel$  and  $u_k^\perp$ , respectively

$$\beta_{kl}^\parallel = u_{k,l}^\parallel, \quad \beta_{kl}^\perp = u_{k,l}^\perp. \quad (4)$$

The constitutive relations between the stresses and distortions are

$$\sigma_{ij}^\parallel = C_{ijkl}\beta_{kl}^\parallel + D_{ijkl}\beta_{kl}^\perp, \quad (5)$$

$$\sigma_{ij}^\perp = D_{klij}\beta_{kl}^\parallel + E_{ijkl}\beta_{kl}^\perp, \quad (6)$$

where  $C_{ijkl}$  is the tensor of the elastic moduli of phonons,  $E_{ijkl}$  is the tensor of the elastic moduli of phasons, and  $D_{ijkl}$  is the tensor of the elastic moduli of the phonon-phason coupling. The constitutive tensors possess the symmetries [18]

$$C_{ijkl} = C_{klij} = C_{ijlk} = C_{jikl}, \quad D_{ijkl} = D_{jikl}, \quad E_{ijkl} = E_{klij}. \quad (7)$$

The symmetries of the tensors of the elastic constants can be simplified according to the specific type of the considered quasicrystal (see e.g. [19, 11]). From Eq. (6) it is obvious that the phason stress tensor  $\sigma_{ij}^\perp$  and phason distortion tensor  $\beta_{kl}^\perp$  are asymmetric tensors and we cannot interchange the indices  $i$  with  $j$  and  $k$  with  $l$ , since the indices  $i$  and  $k$  “live” in the perpendicular space and  $j$  and  $l$  “live” in the material space. In general, if such indices interchange, one gets a symmetry which is sometimes called in physics a “bastard symmetry” [20, 21], because it interrelates two indices of totally different origin; for quasicrystals, namely a “phason” index and a material space index. However, such a “bastard symmetry” is not allowed in the theory of quasicrystals as it can be seen from the symmetries of the tensor  $E_{ijkl}$  in Eq. (7).

If we substitute Eqs. (5), (6) and (4) into Eqs. (2) and (3), we obtain the *coupled inhomogeneous Navier equations for the displacement vectors*

$$C_{ijkl}u_{k,lj}^\parallel + D_{ijkl}u_{k,lj}^\perp = -f_i^\parallel, \quad (8)$$

$$D_{klij}u_{k,lj}^\parallel + E_{ijkl}u_{k,lj}^\perp = -f_i^\perp. \quad (9)$$

In what follows we introduce *the hyperspace notation* for quasicrystals, which is a compact notation in order to describe the fields in the hyperspace. Originally, a compact notation for the mathematical description of coupled fields was introduced by Barnett and Lothe [22] for anisotropic linear piezoelectric crystals. Later, this notation was generalized towards piezoelectric, piezomagnetic and magnetoelectric materials by Alshits et al. [23]. Here, we generalize such a notation towards quasicrystals, so that the phonon and phason fields can be unified in the corresponding extended field in the hyperspace. The components of the extended fields will be denoted by capital letters e.g.  $I, K = 1, \dots, n$ . Therefore, in the hyperspace we have *the extended displacement vector*

$$U_K = \begin{cases} u_k^{\parallel}, & K = 1, 2, 3, \\ u_k^{\perp}, & K = 4, \dots, n, \end{cases} \quad (10)$$

*the extended elastic distortion tensor*

$$B_{Kl} = \begin{cases} \beta_{kl}^{\parallel}, & K = 1, 2, 3, \\ \beta_{kl}^{\perp}, & K = 4, \dots, n, \end{cases} \quad (11)$$

*the extended stress tensor*

$$\Sigma_{Ij} = \begin{cases} \sigma_{ij}^{\parallel}, & I = 1, 2, 3, \\ \sigma_{ij}^{\perp}, & I = 4, \dots, n, \end{cases} \quad (12)$$

*the extended body force vector*

$$F_I = \begin{cases} f_i^{\parallel}, & I = 1, 2, 3, \\ f_i^{\perp}, & I = 4, \dots, n, \end{cases} \quad (13)$$

and *the tensor of the extended elastic moduli*

$$C_{IjKl} = \begin{cases} C_{ijkl}, & I = 1, 2, 3; \quad K = 1, 2, 3, \\ D_{ijkl}, & I = 1, 2, 3; \quad K = 4, \dots, n, \\ D_{kl ij}, & I = 4, \dots, n; \quad K = 1, 2, 3, \\ E_{ijkl}, & I = 4, \dots, n; \quad K = 4, \dots, n, \end{cases} \quad (14)$$

where  $i, j, k, l = 1, 2, 3$ . The tensor  $C_{IjKl}$  retains the symmetry

$$C_{IjKl} = C_{KlIj}. \quad (15)$$

Strictly speaking, the extended tensors appearing in Eqs. (11), (12) and (14) are called double tensor fields [24] or two-point tensors [25], since they have indices in the hyperspace and in the material space. In the linear theory of quasicrystals the material space coincides with the parallel space.

In addition, in the hyperspace notation the constitutive relations (5) and (6) read

$$\Sigma_{Ij} = C_{IjKl} B_{Kl} \quad (16)$$

and the equilibrium conditions (2) and (3) are given by

$$\Sigma_{Ij,j} + F_I = 0. \quad (17)$$

By substituting Eq. (16) into Eq. (17), the equilibrium condition reads in terms of the extended displacement vector  $U_K$

$$C_{IjKl} U_{K,lj} + F_I = 0. \quad (18)$$

This is a Navier-type partial differential equation for the extended displacement vector  $U_K$ .

## 2.2 The generalized three-dimensional elastic Green tensor

In this subsection, we derive the three-dimensional Green tensor and the extended displacement field for an arbitrary external force for quasicrystals in the framework of generalized elasticity theory.

The method of Green functions (see, e.g., [1]) is commonly used to solve linear inhomogeneous partial differential equations like Eq. (18). The *Green tensor*  $G_{KM}(\mathbf{R})$  of the three-dimensional Navier equation (18) is defined by

$$C_{IjKl} G_{KM,lj}(\mathbf{R}) + \delta_{IM} \delta(\mathbf{R}) = 0, \quad (19)$$

where  $\mathbf{R} = \mathbf{x} - \mathbf{x}'$  and  $\delta(\mathbf{R})$  is the three-dimensional Dirac delta function.  $G_{KM}(\mathbf{R})$  represents the displacement in the hyperspace in  $K$ -direction at the point  $\mathbf{R}$  arising from a unit point force in the  $M$ -direction applied at the point  $\mathbf{x}'$ . The Green tensor  $G_{KM}(\mathbf{R})$  satisfies the symmetry relations

$$G_{KM}(\mathbf{R}) = G_{MK}(\mathbf{R}) = G_{KM}(-\mathbf{R}). \quad (20)$$

Using the three-dimensional Fourier transform of the Green tensor

$$G_{KM}(\mathbf{R}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} G_{KM}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{R}} d\mathbf{k} \quad (21)$$

and of the Dirac delta function

$$\delta(\mathbf{R}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} e^{i\mathbf{k} \cdot \mathbf{R}} d\mathbf{k}, \quad (22)$$

Eq. (19) can be transformed to an algebraic equation in the Fourier space

$$C_{IjKl} k_j k_l G_{KM} = \delta_{IM}. \quad (23)$$

If we introduce the unit vector in the Fourier space

$$\boldsymbol{\kappa} = \mathbf{k}/|\mathbf{k}| \quad (24)$$

and the symmetric *Christoffel stiffness tensor* in the hyperspace

$$(\kappa C \kappa)_{IK} = \kappa_j C_{IjKl} \kappa_l = \begin{pmatrix} \kappa_j C_{ijkl} \kappa_l & \kappa_j D_{ijkl} \kappa_l \\ \kappa_j D_{kl ij} \kappa_l & \kappa_j E_{ijkl} \kappa_l \end{pmatrix}, \quad (25)$$

the Green tensor in the Fourier space is written as

$$G_{KM}(\mathbf{k}) = \frac{1}{k^2} (\kappa C \kappa)_{KM}^{-1}, \quad (26)$$

which is a homogeneous function of  $\mathbf{k}$  of degree  $-2$ . The matrix  $(\kappa C \kappa)_{KM}^{-1}$  is the inverse of  $(\kappa C \kappa)_{KM}$  and is given by

$$(\kappa C \kappa)_{KM}^{-1} = \frac{A_{KM}(\boldsymbol{\kappa})}{D(\boldsymbol{\kappa})}, \quad (27)$$

where  $D(\boldsymbol{\kappa})$  and  $A_{KM}(\boldsymbol{\kappa})$  are the determinant and the adjoint of the matrix  $(\kappa C \kappa)_{KM}$ , respectively. Substituting Eq. (26) into Eq. (21), the three-dimensional Fourier integral can be reduced to a line integral along the unit circle in the plane orthogonal to  $\mathbf{R}$  (see Appendix A and [4, 6, 16])

$$\int_{-\infty}^{\infty} G_{KM}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{R}} d\mathbf{k} = \frac{\pi}{R} \int_0^{2\pi} G_{KM}(\mathbf{n}) d\phi, \quad (28)$$

where  $\mathbf{n}$  is a unit vector “scanning” the circle of integration and remaining orthogonal to  $\mathbf{R}$ , thus  $\mathbf{n} \cdot \mathbf{R} = 0$ . In this way, the Green tensor (21) can be written in the form (see Appendix A)

$$G_{KM}(\mathbf{R}) = \frac{1}{8\pi^2 R} \int_0^{2\pi} (n C n)_{KM}^{-1} d\phi. \quad (29)$$

Here,  $\mathbf{n}$  is a function of  $\phi$ . Eq. (29) is *the three-dimensional elastic Green tensor for quasicrystals*. The Green tensor (29) is the generalization of the Green tensor of general anisotropic elasticity (see, e.g., [4, 5, 6, 17, 16, 26]) towards quasicrystals. The integral in Eq. (29) can be computed by standard numerical methods, when  $C_{IjKm}$  is given (see, e.g., [5, 15]) and therefore it is well suited to rapid and accurate numerical integration. The numerical calculation of the Green tensor function of an infinite quasicrystalline medium with general anisotropy can be reduced to the application of standard numerical codes. The elastic Green tensor  $G_{KM}(\mathbf{R})$  can be decomposed into its phonon and phason parts

$$G_{KM}(\mathbf{R}) = \begin{pmatrix} G_{km}^{\parallel\parallel}(\mathbf{R}) & G_{km}^{\parallel\perp}(\mathbf{R}) \\ G_{km}^{\perp\parallel}(\mathbf{R}) & G_{km}^{\perp\perp}(\mathbf{R}) \end{pmatrix} \quad (30)$$

and has the following physical interpretations:

- $G_{km}^{\parallel\parallel}(\mathbf{R})$  = phonon displacement at  $\mathbf{x}$  in the direction  $x_k$  due to a unit phonon point force at  $\mathbf{x}'$  in the  $x_m$  direction;
- $G_{km}^{\parallel\perp}(\mathbf{R})$  = phonon displacement at  $\mathbf{x}$  in the direction  $x_k$  due to a unit phason point force at  $\mathbf{x}'$  in the  $x_m$  direction;
- $G_{km}^{\perp\parallel}(\mathbf{R})$  = phason displacement at  $\mathbf{x}$  in the direction  $x_k$  due to a unit phonon point force at  $\mathbf{x}'$  in the  $x_m$  direction;
- $G_{km}^{\perp\perp}(\mathbf{R})$  = phason displacement at  $\mathbf{x}$  in the direction  $x_k$  due to a unit phason point force at  $\mathbf{x}'$  in the  $x_m$  direction.

The solution of the Green tensor in quasicrystalline materials can be applied to calculate phonon and phason fields caused by an external or internal force. For an arbitrary extended force  $F_M$ , the particular solution of Eq. (18) is written as

$$U_K(\mathbf{x}) = G_{KM} * F_M, \quad (31)$$

where the symbol  $*$  denotes the three-dimensional spatial convolution. Using the Green tensor (29), Eq. (31) gives *the extended displacement vector for an arbitrary extended force  $F_M$  in elasticity theory of quasicrystals*

$$U_K(\mathbf{x}) = \frac{1}{8\pi^2} \int_V \frac{F_M(\mathbf{x}')}{R} \left( \int_0^{2\pi} (nCn)_{KM}^{-1} d\phi \right) dV'. \quad (32)$$

For instance, for a Kelvin-type force, that is  $F_M(\mathbf{R}) = f_M \delta(\mathbf{R})$  with constant magnitude  $f_M$ , Eq. (32) reduces to

$$U_K(\mathbf{x}) = G_{KM}(\mathbf{x}) f_M = \frac{f_M}{8\pi^2 r} \int_0^{2\pi} (nCn)_{KM}^{-1} d\phi. \quad (33)$$

Eq. (33) is *the Kelvin-type force solution for quasicrystals*.

## 3 Dislocation theory of quasicrystals

### 3.1 Basic framework, the field equations and their solutions

First, the basic framework for dislocations in quasicrystals is presented. Next, we give the field equations for the extended displacement vector and the extended elastic distortion tensor and we derive their particular solutions. For a review of the physics of dislocations in quasicrystals, we refer to Feuerbacher [27] and Wang and Hu [28].

In general, if dislocations are present, the theory of compatible elasticity modifies to the theory of incompatible elasticity incorporating plastic fields. For incompatible elasticity theory of quasicrystals we refer to Ding et al. [13], Hu et al. [19] and Agiasofitou et al. [29]. In the presence of dislocations inside the medium, the displacement



gradient is usually decomposed into *the elastic distortion tensors*  $\beta_{ij}^{\parallel}$ ,  $\beta_{ij}^{\perp}$ , and *the plastic distortion tensors*  $\beta_{ij}^{\parallel P}$ ,  $\beta_{ij}^{\perp P}$ , according to

$$u_{i,j}^{\parallel} = \beta_{ij}^{\parallel} + \beta_{ij}^{\parallel P}, \quad u_{i,j}^{\perp} = \beta_{ij}^{\perp} + \beta_{ij}^{\perp P}. \quad (34)$$

The incompatibility of the elastic and plastic parts gives rise to the existence of dislocation density tensors. *The phonon and phason dislocation density tensors*  $\alpha_{ij}^{\parallel}$  and  $\alpha_{ij}^{\perp}$ , respectively, are defined in terms of the elastic distortion tensors

$$\alpha_{ij}^{\parallel} = \epsilon_{jkl} \beta_{il,k}^{\parallel}, \quad \alpha_{ij}^{\perp} = \epsilon_{jkl} \beta_{il,k}^{\perp} \quad (35)$$

or in terms of the plastic distortion tensors

$$\alpha_{ij}^{\parallel} = -\epsilon_{jkl} \beta_{il,k}^{\parallel P}, \quad \alpha_{ij}^{\perp} = -\epsilon_{jkl} \beta_{il,k}^{\perp P}, \quad (36)$$

where  $\epsilon_{jkl}$  is the three-dimensional Levi-Civita tensor. In our notation, the first index of the dislocation density tensor (Eq. (36)) shows the orientation of the Burgers vector and the second index shows the direction of the dislocation line. The dislocation density tensors satisfy the following Bianchi identities

$$\alpha_{ij,j}^{\parallel} = 0, \quad \alpha_{ij,j}^{\perp} = 0, \quad (37)$$

which mean that dislocations cannot end inside the quasicrystalline medium.

In the absence of external forces, the field equations for the phonon and phason displacement fields are (see, e.g., [13, 29, 30])

$$C_{ijkl} u_{k,lj}^{\parallel} + D_{ijkl} u_{k,lj}^{\perp} = C_{ijkl} \beta_{kl,j}^{\parallel P} + D_{ijkl} \beta_{kl,j}^{\perp P}, \quad (38)$$

$$D_{klij} u_{k,lj}^{\parallel} + E_{ijkl} u_{k,lj}^{\perp} = D_{klij} \beta_{kl,j}^{\parallel P} + E_{ijkl} \beta_{kl,j}^{\perp P}, \quad (39)$$

where the plastic distortion tensors play the role of the sources for the displacement vectors. The corresponding field equations for the elastic distortion tensors are of the form [30]

$$C_{ijkl} \beta_{km,lj}^{\parallel} + D_{ijkl} \beta_{km,lj}^{\perp} = \epsilon_{lmp} (C_{ijkl} \alpha_{kp,j}^{\parallel} + D_{ijkl} \alpha_{kp,j}^{\perp}), \quad (40)$$

$$D_{klij} \beta_{km,lj}^{\parallel} + E_{ijkl} \beta_{km,lj}^{\perp} = \epsilon_{lmp} (D_{klij} \alpha_{kp,j}^{\parallel} + E_{ijkl} \alpha_{kp,j}^{\perp}), \quad (41)$$

where the dislocation density tensors are the source fields.

A dislocation in a quasicrystal can be considered as a “hyperdislocation” in the hyperlattice by means of a generalized Volterra process. Because the hyperlattice is periodic, the generalized Volterra process can be understood as insertion or removal of a hyper-halfplane (e.g., [27]). The Burgers vector of the “hyperdislocation” consists of phonon and phason components

$$b_I = (b_i^{\parallel}, b_i^{\perp}) \in E_{\parallel} \oplus E_{\perp}. \quad (42)$$

A “hyperdislocation” is a line defect in a quasicrystal characterized by the Burgers vector and the direction of the dislocation line in the material space. It should be noted

that for a perfect dislocation in a quasicrystal, both components  $\mathbf{b}^{\parallel}$  and  $\mathbf{b}^{\perp}$  are non-zero and the Burgers vector  $\mathbf{b}$  is a lattice vector in the hyperspace. If the phason component  $\mathbf{b}^{\perp}$  is zero, then there exist a stacking fault along the cutting surface of the generalized Volterra process, and this dislocation represents a partial dislocation, since  $\mathbf{b}^{\parallel}$  alone is not a lattice vector in the hyperspace (see [28]).

Using the hyperspace notation, we can write *the extended plastic distortion tensor*

$$B_{Kl}^P = \begin{cases} \beta_{kl}^{\parallel P}, & K = 1, 2, 3, \\ \beta_{kl}^{\perp P}, & K = 4, \dots, n, \end{cases} \quad (43)$$

and *the extended dislocation density tensor*

$$A_{Kl} = \begin{cases} \alpha_{kl}^{\parallel}, & K = 1, 2, 3, \\ \alpha_{kl}^{\perp}, & K = 4, \dots, n. \end{cases} \quad (44)$$

With the definitions (43) and (44), Eqs. (34)–(36) can be respectively written

$$U_{I,j} = B_{Ij} + B_{Ij}^P \quad (45)$$

and

$$A_{Ij} = \epsilon_{jkl} B_{Il,k}, \quad A_{Ij} = -\epsilon_{jkl} B_{Il,k}^P. \quad (46)$$

Moreover, the Bianchi identity is reduced (in the hyperspace) to

$$A_{Kl,l} = 0. \quad (47)$$

In the hyperspace, *the field equation for the extended displacement vector*  $U_K$  (see Eqs. (38) and (39)) is written as

$$C_{IjKl} U_{K,lj} = C_{IjKl} B_{Kl,j}^P, \quad (48)$$

which is an inhomogeneous Navier equation. If we compare Eqs. (48) and (18), we may introduce an “internal force caused by dislocations” as

$$F_I = -C_{IjKl} B_{Kl,j}^P. \quad (49)$$

The force (49) is a fictitious body force. From Eq. (49), the internal phason force density due to dislocations reads (see also [13, 19])

$$f_i^{\perp} = -D_{klij} \beta_{kl,j}^{\parallel P} - E_{ijkl} \beta_{kl,j}^{\perp P}, \quad (50)$$

which is non-zero if dislocations exist in the quasicrystalline medium. Thus, Eq. (50) is an example of a phason force caused by the gradient of the plastic fields of dislocations. The particular solution of Eq. (48) following Eq. (31) reads

$$U_I = G_{IJ} * F_J = -C_{JkLm} G_{IJ} * B_{Lm,k}^P = -C_{JkLm} G_{IJ,k} * B_{Lm}^P, \quad (51)$$

where  $G_{IJ}$  is given by Eq. (29). Eq. (51) gives *the extended displacement vector in a quasicrystal that has experienced an extended plastic distortion*  $B_{Lm}^P$ . It is important to

note that Eq. (51) is the Volterra-type representation of the displacement vector  $U_I$  for an arbitrary plastic distortion tensor  $B_{Lm}^P$ .

The field equations (40) and (41) simplify in the hyperspace notation to the following *field equation for the extended elastic distortion tensor*

$$C_{IjKl}B_{Km,lj} = \epsilon_{lmn} C_{IjKl}A_{Kn,j}, \quad (52)$$

which is a tensorial Navier equation. The particular solution of Eq. (52) is given by

$$B_{Im} = \epsilon_{mnr} C_{JkLn} G_{IJ,k} * A_{Lr}. \quad (53)$$

Eq. (53) is *the generalization of the so-called Mura-Willis formula* [31, 32] *towards quasicrystals*. Once we know the extended elastic distortion tensor we can calculate the extended stress tensor by means of Eq. (16), that is

$$\Sigma_{Ps} = C_{PsIm} \epsilon_{mnr} C_{JkLn} G_{IJ,k} * A_{Lr}. \quad (54)$$

### 3.2 The generalized Burgers equation for arbitrary sources

In this subsection, we derive an alternative expression for the solution of the extended displacement vector  $U_I$ , using a straightforward method introduced by Lazar and Kirchner [17]. This method gives directly the Burgers equation for arbitrary plastic distortions and dislocation densities. It is mainly based on three steps: the linear decomposition of the total distortion into the elastic and plastic distortions, the Green function of the Poisson equation and the Mura-Willis formula. Using this method, the solution of the extended displacement field can be decomposed into a purely geometric part depending on the plastic distortion and a part depending on the tensor of the elastic constants and the dislocation density. Therefore, it is not necessary to solve the inhomogeneous Navier equation (48) in order to extract a purely geometric part from it.

The divergence from the right of Eq. (45) gives the following Poisson equation for the displacement field  $U_I$

$$\Delta U_I = B_{Im,m}^P + B_{Im,m}. \quad (55)$$

Using the three-dimensional Green function of the Poisson equation (e.g., [1, 33])

$$\Delta G = \delta(\mathbf{R}), \quad G = -\frac{1}{4\pi R}, \quad (56)$$

the solution  $U_I$  of Eq. (55) is given by

$$U_I = -[B_{Im,m}^P + B_{Im,m}] * \frac{1}{4\pi R}. \quad (57)$$

The above equation using the generalized Mura-Willis formula (53) is written

$$U_I = -B_{Im,m}^P * \frac{1}{4\pi R} - [\epsilon_{mnr} C_{JkLn} G_{IJ,k} * A_{Lr}] * \frac{1}{4\pi R}. \quad (58)$$

Using the associative law for the convolution, Eq. (58) can be rewritten as

$$U_I = -B_{Im,m}^P * \frac{1}{4\pi R} - \epsilon_{mnr} C_{JkLn} \left[ G_{IJ,km} * \frac{1}{4\pi R} \right] * A_{Lr}. \quad (59)$$

The inconvenience of the double convolution in the second term of Eq. (59) can be reduced to a single one. To this aim, we introduce the tensor  $F_{mnIJ}$ , which was originally introduced by Kirchner [34, 35] for anisotropic elasticity (see also [17])

$$F_{mkIJ} = G_{IJ,km} * \frac{1}{4\pi R}. \quad (60)$$

We may call the tensor  $F_{mnIJ}$  as *the potential of the second gradient of the Green tensor*, since it satisfies the Poisson equation

$$\Delta F_{mkIJ} + G_{IJ,km} = 0. \quad (61)$$

Moreover, the following relationships hold

$$F_{mkIJ,m} + G_{IJ,k} = 0, \quad F_{mkIJ,k} + G_{IJ,m} = 0 \quad (62)$$

and

$$F_{mkIJ,mk} + \Delta G_{IJ} = 0. \quad (63)$$

In addition,  $F_{mnIJ}$  possesses the symmetry properties

$$F_{mkIJ} = F_{kmIJ} = F_{mkJI} \quad (64)$$

and

$$F_{mkIJ}(\mathbf{R}) = F_{mkIJ}(-\mathbf{R}). \quad (65)$$

Using Eq. (19), Eq. (60) becomes

$$C_{JkLm} F_{mkIJ} = -\frac{1}{4\pi R} \delta_{IL}. \quad (66)$$

The Fourier transform of  $F_{mnIJ}$  is

$$F_{mkIJ}(\mathbf{k}) = -\frac{1}{k^2} \kappa_m \kappa_k (\kappa C \kappa)_{IJ}^{-1}. \quad (67)$$

Like the Fourier transform of the Green tensor (26),  $F_{mnIJ}$  in Eq. (67) varies like  $k^{-2}$ . Thus, its three-dimensional inverse Fourier transform for  $\mathbf{n} \cdot \mathbf{R} = 0$  reduces to a one-dimensional integration in the angle  $\phi$

$$\int_{-\infty}^{\infty} F_{mkIJ}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{R}} d\mathbf{k} = \frac{\pi}{R} \int_0^{2\pi} F_{mkIJ}(\mathbf{n}) d\phi, \quad (68)$$

where  $\mathbf{n}$  is a unit vector “scanning” the circle of integration and remaining orthogonal to  $\mathbf{R}$ . Consequently, the three-dimensional potential of the second gradient of the Green tensor is given by

$$F_{mkIJ}(\mathbf{R}) = -\frac{1}{8\pi^2 R} \int_0^{2\pi} n_m n_k (nCn)_{IJ}^{-1} d\phi. \quad (69)$$

Like Eq. (29), Eq. (69) is well suited to rapid and accurate numerical integration. Moreover, comparing Eqs. (29) and (69), we obtain the following important relation

$$\delta_{mk} F_{mkIJ} = -G_{IJ}. \quad (70)$$

Hence, Eq. (59) via the definition (60) reduces to a single convolution integral

$$U_I = -B_{Im,m}^P * \frac{1}{4\pi R} - \epsilon_{rmn} C_{JkLn} F_{mkIJ} * A_{Lr}, \quad (71)$$

where  $F_{mkIJ}$  is given by Eq. (69). Eq. (71) is *the generalized Burgers equation for arbitrary sources*. It represents *the solution of the extended displacement vector in dislocation theory*, when  $B_{IJ}^P$  and  $A_{Ij}$  are given and is valid for any distribution of dislocations. The plastic distortion tensor  $B_{IJ}^P$  and the corresponding dislocation density tensor  $A_{Ij}$  can represent discrete dislocations (straight dislocations, dislocation loops) or a continuous distribution of dislocations. It is worth noting that the first term in Eq. (71) is a purely geometric part because it does not depend on the properties of the medium. Only the second part depends on the properties of the material due to the appearance of the tensor of elastic constants  $C_{JkLn}$  and the tensor  $F_{mkIJ}$ . The structure of Eq. (71) is a direct consequence of the decomposition of the total distortion tensor into an elastic and a plastic part (see Eq. (45)). Due to this clear decomposition of the displacement vector into a geometric part determined by the plastic distortion and a part depending on the elastic coefficients and the dislocation density tensor, the representation of the displacement field (71) is more suitable than the Volterra-type representation (51) in solving dislocation problems.

### 3.3 The Eshelby stress tensor and the Peach-Koehler force

We derive here quantities that play an important role in defect mechanics and in the so-called Eshelbian mechanics [36, 37, 38, 39]; namely the Eshelby stress tensor, the Peach-Koehler force and the  $J$ -integral. In general, the  $J$ -integral [40, 41, 42] is important for dislocations, cracks and fracture mechanics, especially for a dislocation based fracture mechanics.

We start with a direct derivation of the Eshelby stress tensor of quasicrystals following Lazar and Kirchner [17]. If we multiply Eq. (46) by  $\epsilon_{jkl}$ , we obtain

$$B_{Ik,j} - B_{Ij,k} = \epsilon_{jkl} A_{Il}, \quad (72)$$

which multiplied by  $\Sigma_{Ik}$  gives

$$W_{,j} - \Sigma_{Ik} B_{Ij,k} = \epsilon_{jkl} \Sigma_{Ik} A_{Il}, \quad (73)$$

where the elastic strain energy density (for the unlocked state) is given by

$$W = \frac{1}{2} \Sigma_{Ij} B_{Ij} = \frac{1}{2} \sigma_{ij}^{\parallel} \beta_{ij}^{\parallel} + \frac{1}{2} \sigma_{ij}^{\perp} \beta_{ij}^{\perp}. \quad (74)$$

Using Eq. (17) for vanishing extended body forces, we obtain

$$[W \delta_{jk} - \Sigma_{Ik} B_{Ij}]_{,k} = \epsilon_{jkl} \Sigma_{Ik} A_{Il}. \quad (75)$$

In the brackets on the left hand side of Eq. (75), the *Eshelby stress tensor for quasicrystals* [29] appears

$$P_{jk} = W \delta_{jk} - \Sigma_{Ik} B_{Ij} = W \delta_{jk} - \sigma_{lk}^{\parallel} \beta_{lj}^{\parallel} - \sigma_{lk}^{\perp} \beta_{lj}^{\perp} \quad (76)$$

and it consists of phonon and phason fields. The trace of the Eshelby stress tensor (76) reads

$$P_{jj} = \frac{1}{2} \Sigma_{Ij} B_{Ij} = \frac{1}{2} (\sigma_{ij}^{\parallel} \beta_{ij}^{\parallel} + \sigma_{ij}^{\perp} \beta_{ij}^{\perp}). \quad (77)$$

The skew-symmetric part of the Eshelby stress tensor (76) is given by

$$\epsilon_{ijk} P_{jk} = \epsilon_{ijk} \Sigma_{Ij} B_{Ik} = \epsilon_{ijk} (\sigma_{lj}^{\parallel} \beta_{lk}^{\parallel} + \sigma_{lj}^{\perp} \beta_{lk}^{\perp}). \quad (78)$$

It is known that the Eshelby stress tensor stems from spatial translational transformations in the material space and is the static part of the energy-momentum tensor. The source term on the right hand side of Eq. (75) is the so-called *Peach-Koehler force density* [29]

$$f_j^{\text{PK}} = \epsilon_{jkl} \Sigma_{Ik} A_{Il} = \epsilon_{jkl} (\sigma_{ik}^{\parallel} \alpha_{il}^{\parallel} + \sigma_{ik}^{\perp} \alpha_{il}^{\perp}), \quad (79)$$

which consists of a phonon stress-dislocation density part and a phason stress-dislocation density part. Thus, Eq. (75) is a translational material balance law, where the divergence of the Eshelby stress tensor (76) is balanced by the Peach-Koehler force density (79),

$$P_{jk,k} = f_j^{\text{PK}}. \quad (80)$$

The integral form of the balance law (80) gives the so-called *J-integral for dislocations in quasicrystals*

$$J_j := \int_V P_{jk,k} dV = \int_S P_{jk} dS_k = \int_S [W \delta_{jk} - \Sigma_{Ik} B_{Ij}] dS_k = \int_V f_j^{\text{PK}} dV, \quad (81)$$

where the Gauss theorem has been used. From Eq. (81) it can be seen that the *J-integral for dislocations* is equivalent to the Peach-Koehler force (see also [43, 44, 42]).

### 3.4 The stress function tensor

Herein, we deduce the stress function tensor of first order for the self-stresses of general dislocations. Using the method of the stress function tensor of first order (e.g., [45]), the equilibrium condition (17) is fulfilled automatically for vanishing external forces.

For the self-stresses caused by dislocations, that means that the external forces are zero, the equilibrium condition (17) can be satisfied by deriving the asymmetric stress  $\Sigma_{Ij}$  from an asymmetric *stress function tensor*  $\Phi_{Ij}$ , which is a stress function tensor of first order, as follows

$$\Sigma_{Ij} = \epsilon_{jkl} \Phi_{Il,k} . \quad (82)$$

For the stress (82), the equilibrium condition (17) for vanishing forces,  $\Sigma_{Ij,j} = 0$ , is automatically satisfied. Now, we perform the curl on the right index of the stress tensor (82)

$$\epsilon_{mnj} \Sigma_{Ij,n} = \epsilon_{mnj} \epsilon_{jkl} \Phi_{Il,kn} = \Phi_{Il,lm} - \Delta \Phi_{Im} . \quad (83)$$

Imposing the side condition (see, e.g., [45])

$$\Phi_{Ij,j} = 0 , \quad (84)$$

we find the following Poisson equation for the stress function tensor

$$\Delta \Phi_{Ij} = -\epsilon_{jkl} \Sigma_{Il,k} . \quad (85)$$

Using Eq. (56), we find the solution

$$\Phi_{Ij} = \epsilon_{jkl} \Sigma_{Il,k} * \frac{1}{4\pi R} , \quad (86)$$

which with the help of the constitutive relation (16) becomes

$$\Phi_{Ij} = \epsilon_{jkl} C_{IlMn} B_{Mn,k} * \frac{1}{4\pi R} . \quad (87)$$

Substituting Eq. (53) into Eq. (87) and using the associative law for the convolution (see, e.g., [1]), we obtain

$$\Phi_{Ij} = \left[ \epsilon_{jkl} C_{IlMn} \epsilon_{npq} C_{RsTp} G_{MR,ks} * \frac{1}{4\pi R} \right] * A_{Tq} . \quad (88)$$

It is easy to check that Eq. (88) satisfies the side condition (84) and reproduces the extended stress tensor (54) by inserting Eq. (88) into Eq. (82). Moreover, one can see that in Eq. (88) the potential of the second gradient of the Green tensor  $F_{mkIJ}$  (Eq. (60)) is appearing. Consequently, Eq. (88) is rewritten as

$$\Phi_{Ij} = \epsilon_{jkl} C_{IlMn} \epsilon_{npq} C_{RsTp} F_{skMR} * A_{Tq} . \quad (89)$$

Eq. (89) gives the *stress function tensor for dislocations in quasicrystals* and it holds for discrete dislocations as well as for a continuous distribution of dislocations. Furthermore, the product of the two Levi-Civita tensors may be factored out and if we use Eqs. (47) and (66), Eq. (89) simplifies to

$$\Phi_{Ij} = C_{IlTl} \frac{1}{4\pi R} * A_{Tj} - C_{IlTj} \frac{1}{4\pi R} * A_{Tl} + C_{IlMk} C_{RsTl} F_{skMR} * A_{Tj} - C_{IlMk} C_{RsTj} F_{skMR} * A_{Tl} . \quad (90)$$

### 3.5 The interaction energy

We calculate the interaction energy between two general dislocations, that means discrete dislocations or a continuous distribution of dislocations.

The interaction energy between two dislocations is defined by

$$W^{(AB)} = \int_V \Sigma_{Ij}^{(B)} B_{Ij}^{(A)} dV, \quad (91)$$

where  $\Sigma_{Ij}^{(A)}$ ,  $\Sigma_{Ij}^{(B)}$  are the (asymmetric) extended stress tensors and  $B_{Ij}^{(A)}$ ,  $B_{Ij}^{(B)}$  are the extended elastic distortions of the individual dislocations. Expressing the stresses in terms of the corresponding stress function tensors  $\Phi_{Ij}^{(A)}$ ,  $\Phi_{Ij}^{(B)}$  (see Eq. (82)), using integration by parts and neglecting the surface terms at infinity, we obtain

$$W^{(AB)} = \int_V (\epsilon_{jkl} \Phi_{Il,k}^{(B)}) B_{Ij}^{(A)} dV = \int_V \Phi_{Il}^{(B)} (\epsilon_{lkj} B_{Ij,k}^{(A)}) dV = \int_V \Phi_{Ij}^{(B)} A_{Ij}^{(A)} dV, \quad (92)$$

where  $A_{Ij}^{(A)}$ ,  $A_{Ij}^{(B)}$  are the corresponding extended dislocation densities. If we substitute Eq. (89) into Eq. (92), *the interaction energy between dislocations* reads

$$W^{(AB)} = \int_V \left( [\epsilon_{jkl} C_{IlMn} \epsilon_{npq} C_{RsTp} F_{skMR}] * A_{Tq}^{(B)} \right) A_{Ij}^{(A)} dV. \quad (93)$$

Substituting Eq. (90) into Eq. (92), we take an alternative formula for the interaction energy between dislocations

$$W^{(AB)} = \int_V \left( C_{IlTl} \frac{1}{4\pi R} * A_{Tj}^{(B)} - C_{IlTj} \frac{1}{4\pi R} * A_{Tl}^{(B)} + C_{IlMk} C_{RsTl} F_{skMR} * A_{Tj}^{(B)} - C_{IlMk} C_{RsTj} F_{skMR} * A_{Tl}^{(B)} \right) A_{Ij}^{(A)} dV. \quad (94)$$

### 3.6 Dislocation loops

The obtained general formulas of the previous subsections are applied to the case of dislocation loops deducing in this way the generalized Burgers equation and all other dislocation key-formulas for loops.

For a dislocation loop  $L$ , the extended dislocation density and the extended plastic distortion tensors are of the form (see, e.g., [30])

$$A_{Ij} = b_I \delta_j(L) = b_I \oint_L \delta(\mathbf{x} - \mathbf{x}') dL'_j, \quad (95)$$

$$B_{Ij}^P = -b_I \delta_j(S) = -b_I \int_S \delta(\mathbf{x} - \mathbf{x}') dS'_j, \quad (96)$$

where  $b_I$  is the Burgers vector in the hyperspace,  $dL'_j$  denotes the dislocation line element at  $\mathbf{x}'$  and  $dS'_j$  is the dislocation loop area. The surface  $S$  is the “cap” over the dislocation line  $L$ . The surface  $S$  represents the area swept by the loop  $L$  during its motion and may be called *the dislocation surface*. The plastic distortion caused



by a dislocation loop is concentrated at the surface  $S$ . Thus, the surface  $S$  is what determines the history of the plastic distortion of a dislocation loop (see, e.g, [46, 31]). Here,  $\delta_j(L)$  is the Dirac delta function for a closed curve  $L$  and  $\delta_j(S)$  is the Dirac delta function for a surface  $S$  whose boundary is  $L$ . For the forthcoming calculations we need the following relations [31]

$$\int_V \delta_k(S') f(\mathbf{x} - \mathbf{x}') dV' = \int_S f(\mathbf{x} - \mathbf{x}') dS'_k, \quad (97)$$

$$\int_V \delta_k(L') f(\mathbf{x} - \mathbf{x}') dV' = \oint_L f(\mathbf{x} - \mathbf{x}') dL'_k. \quad (98)$$

### 3.6.1 Generalized Burgers equation

Here, we find the expression of the extended displacement vector (71) for a dislocation loop, providing in this way the generalized Burgers equation.

We start with the calculation of the first term of Eq. (71), which using the expression of  $B_{Ij}^P$  (Eq. (96)) and the relation (97) becomes

$$B_{Im,m}^P * \frac{1}{4\pi R} = -\frac{b_I}{4\pi} \partial_m \int_V \frac{1}{R} \delta_m(S') dV' = -\frac{b_I}{4\pi} \int_S \partial_m \left( \frac{1}{R} \right) dS'_m = \frac{b_I \Omega}{4\pi}, \quad (99)$$

where *the solid angle*  $\Omega$  is defined by

$$\Omega = - \int_S \partial_m \left( \frac{1}{R} \right) dS'_m = \int_S \frac{R_m}{R^3} dS'_m. \quad (100)$$

The solid angle is the angle under which the loop  $L$  can be seen from the point  $\mathbf{x}$ . It is very useful for the numerical implementation that the solid angle (100) can be transformed into a line integral and a constant contribution [47]

$$\Omega = \oint_L A_k(\mathbf{R}) dL'_k - 4\pi \begin{cases} 1, & \text{if } C \text{ crosses } S \text{ positively,} \\ 0, & \text{if } C \text{ does not cross } S, \\ -1, & \text{if } C \text{ crosses } S \text{ negatively.} \end{cases} \quad (101)$$

In Eq. (101),  $C$  is a curve, called the “Dirac string”, starting at  $-\infty$  and ending at the origin (for convenience  $C$  is usually chosen to be a straight line) and  $A_k(\mathbf{R})$  is the vector potential of a “magnetic monopole” [48, 49], which is given by

$$A_k(\mathbf{R}) = \epsilon_{klm} \frac{\hat{n}_l R_m}{R(R + R_i \hat{n}_i)}, \quad (102)$$

where  $\hat{n}_i$  is an arbitrary but constant unit vector on  $C$ .

So far, Eq. (71) reads for a dislocation loop

$$U_I(\mathbf{x}) = -\frac{b_I \Omega}{4\pi} - \epsilon_{rmn} C_{JkLn} F_{mkIJ} * A_{Lr}. \quad (103)$$

If we substitute Eqs. (95) and (69) into Eq. (103) and use the relation (98), the final result is given by

$$U_I(\mathbf{x}) = -\frac{b_I \Omega}{4\pi} + \frac{b_L \epsilon_{rmp}}{8\pi^2} \oint_L \frac{1}{R} \left( \int_0^{2\pi} C_{JkLp} n_m n_k (nCn)_{IJ}^{-1} d\phi \right) dL'_r. \quad (104)$$

Eq. (104) is *the generalized Burgers formula for dislocation loops in quasicrystals*. It is obvious that it is the generalization of the Burgers formula of general anisotropic elasticity (see, e.g., [17]) towards the theory of quasicrystals. The extended displacement vector is written as the sum of a line integral plus a purely geometric part. Due to the anisotropy, an integration in  $\phi$  appears in Eq. (104). In the integrand the unit vector  $n_m$ , which is perpendicular to  $\mathbf{R}$ , the expression  $(nCn)_{IJ}^{-1}$  and  $C_{JkLp}n_k$  are functions of  $\phi$ . It is worth noting that there is no need for further numerical differentiation. Due to the simplicity of the result (104), it can be used directly in numerical simulations and discrete dislocation dynamics of quasicrystals.

### 3.6.2 Other dislocation key-formulas for loops

In this subsection, we derive the generalizations of Mura-Willis equation, Peach-Koehler stress formula, Volterra equation, Peach-Koehler force and stress function tensor for a dislocation loop towards the theory of quasicrystals. Moreover, the explicit formula of the interaction energy between two dislocation loops in quasicrystalline materials is also deduced.

If we substitute Eq. (95) into Eq. (53) and perform the convolution using Eq. (98), we find *the generalized Mura-Willis equation for a dislocation loop in quasicrystals*

$$B_{Im}(\mathbf{x}) = \oint_L \epsilon_{mnr} C_{JkLn} b_L G_{IJ,k}(\mathbf{R}) dL'_r. \quad (105)$$

In addition, by inserting Eq. (95) into Eq. (54) and calculate the convolution by the help of Eq. (98), the extended stress tensor of a dislocation loop follows

$$\Sigma_{Ps}(\mathbf{x}) = C_{PsIm} \oint_L \epsilon_{mnr} C_{JkLn} b_L G_{IJ,k}(\mathbf{R}) dL'_r, \quad (106)$$

which is *the generalization of the Peach-Koehler stress formula* towards the theory of quasicrystals.

Once the extended distortion tensor  $B_{Im}$  (Eq. (105)) and the extended stress tensor  $\Sigma_{Ps}$  (Eq. (106)) are known for a dislocation loop, then *the Eshelby stress tensor for a dislocation loop* can be easily calculated by substituting Eqs. (105) and (106) into Eq. (76).

By substituting the extended plastic distortion tensor (96) into Eq. (51) and using Eq. (97) in order to calculate the convolution, we obtain *the generalized Volterra equation for a dislocation loop in quasicrystals*

$$U_I(\mathbf{x}) = \int_S C_{JkLm} b_L G_{IJ,k}(\mathbf{R}) dS'_m. \quad (107)$$

Eqs. (81) and (79) using the relations (95) and (98) give the  $J$ -integral for a dislocation loop which is equivalent to *the Peach-Koehler force for a dislocation loop  $L$  interacting with the stress field  $\Sigma_{Ik}$*

$$J_j \equiv F_j^{\text{PK}} = \int_V f_j^{\text{PK}} dV = \oint_L \epsilon_{jkl} b_l \Sigma_{Ik} dL'_l. \quad (108)$$

Next, we consider two dislocation loops  $L^{(A)}$  and  $L^{(B)}$  with Burgers vectors  $b_I^{(A)}$  and  $b_I^{(B)}$ , respectively. If we substitute Eq. (106) into Eq. (108), *the Peach-Koehler force between the dislocation loop  $L^{(A)}$  in the stress field caused by the dislocation loop  $L^{(B)}$*  reads

$$F_j^{\text{PK}} = \oint_{L^{(A)}} \oint_{L^{(B)}} b_I^{(A)} b_T^{(B)} [\epsilon_{jkl} C_{IkMn} \epsilon_{npq} C_{RsTp} G_{MR,s}(\mathbf{R})] dL_q^{(B)} dL_l^{(A)}, \quad (109)$$

where  $R = |\mathbf{x}^{(A)} - \mathbf{x}^{(B)}|$  is the distance between two points of the dislocation loops  $L^{(A)}$  and  $L^{(B)}$ .

In Eqs. (105)–(107) and Eq. (109), the gradient of the Green tensor is given by (see Appendix B)

$$G_{IJ,k}(\mathbf{R}) = -\frac{1}{8\pi^2 R^2} \int_0^{2\pi} \left( \tau_k (nCn)_{IJ}^{-1} - n_k (nCn)_{IM}^{-1} [(nC\tau)_{MN} + (\tau Cn)_{MN}] (nCn)_{NJ}^{-1} \right) d\phi, \quad (110)$$

where  $\boldsymbol{\tau} = \mathbf{R}/R$  is the unit vector along  $\mathbf{R}$ .

Using Eqs. (69) and (95), Eq. (89) becomes

$$\Phi_{Ij}(\mathbf{x}) = \epsilon_{jkl} C_{IkMn} \epsilon_{npq} C_{RsTp} \frac{b_T}{8\pi^2} \oint_L \frac{1}{R} \left( \int_0^{2\pi} n_l n_s (nCn)_{MR}^{-1} d\phi \right) dL'_q. \quad (111)$$

Eq. (111) gives *the stress function tensor for a dislocation loop in quasicrystals*. The integration in  $\phi$  is to be done around  $\mathbf{R}$ .

Using Eqs. (95) and (98), the interaction energy (92) becomes

$$W^{(AB)} = \oint_{L^{(A)}} b_I^{(A)} \Phi_{Ij}^{(B)} dL_j^{(A)}. \quad (112)$$

Substituting Eq. (111) into Eq. (112), we obtain *the interaction energy between two dislocation loops in quasicrystals*

$$W^{(AB)} = \frac{b_I^{(A)} b_T^{(B)}}{8\pi^2} \oint_{L^{(A)}} \oint_{L^{(B)}} \epsilon_{jkl} C_{IkMn} \epsilon_{npq} C_{RsTp} \frac{1}{R} \left( \int_0^{2\pi} n_l n_s (nCn)_{MR}^{-1} d\phi \right) dL_q^{(B)} dL_j^{(A)}. \quad (113)$$

Moreover, Eq. (113) may be re-written as follows

$$W^{(AB)} = b_I^{(A)} b_T^{(B)} M_{IT}^{(AB)}, \quad (114)$$

where

$$M_{IT}^{(AB)} = \frac{1}{8\pi^2} \oint_{L^{(A)}} \oint_{L^{(B)}} \epsilon_{jkl} C_{IkMn} \epsilon_{npq} C_{RsTp} \frac{1}{R} \left( \int_0^{2\pi} n_l n_s (nCn)_{MR}^{-1} d\phi \right) dL_q^{(B)} dL_j^{(A)}, \quad (115)$$

is the so-called “dislocation mutual inductance” tensor (see [45, 46, 50]), which is in general asymmetric.

Furthermore, substituting Eq. (95) into Eq. (94), we obtain an explicit formula for the interaction energy between two loops, which lends itself readily to numerical implementation

$$\begin{aligned}
W^{(AB)} = & b_I^{(A)} b_T^{(B)} \left( C_{ITl} \oint_{L^{(A)}} \oint_{L^{(B)}} \frac{1}{4\pi R} dL_j^{(B)} dL_j^{(A)} - C_{ITj} \oint_{L^{(A)}} \oint_{L^{(B)}} \frac{1}{4\pi R} dL_l^{(B)} dL_j^{(A)} \right. \\
& \left. + C_{IMk} C_{RsTl} \oint_{L^{(A)}} \oint_{L^{(B)}} F_{skMR}(R) dL_j^{(B)} dL_j^{(A)} - C_{IMk} C_{RsTj} \oint_{L^{(A)}} \oint_{L^{(B)}} F_{skMR}(R) dL_l^{(B)} dL_j^{(A)} \right). \quad (116)
\end{aligned}$$

All the aforementioned dislocation key-formulas using Eq. (110) can be implemented into numerical codes in a straightforward manner, since the appearing integrals are “well-behaved” functions (e.g., [5]).

## 4 Conclusion

In this work, fundamental aspects of generalized elasticity and dislocation theory of quasicrystals have been investigated. Generalized elasticity theory of quasicrystals is a theory of coupled phonon and phason fields. First, we have pointed out the calculation of the three-dimensional elastic Green tensor for one-, two-, and three-dimensional quasicrystals. Second, using the Green tensor, all the dislocation key-formulas known from anisotropic elasticity, that is Burgers formula, Mura-Willis formula, Volterra formula, Peach-Koehler stress formula, Peach-Koehler force, Eshelby stress tensor, the  $J$ -integral and the interaction energy have been generalized towards the theory of quasicrystals. The obtained key-formulas are important for dislocation-based plasticity since a dislocation is the elementary carrier of plasticity, and for dislocation based fracture mechanics of quasicrystals. Moreover, another advantage of the obtained results is that they can be used to build a discrete dislocation dynamics of quasicrystals similar to the discrete dislocation dynamics of anisotropic crystals (see, e.g., [51]).

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## A The elastic Green tensor

In this Appendix, we give some details concerning the calculation of the three-dimensional Green tensor (29) using the inverse Fourier transform

$$G_{KM}(\mathbf{R}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{1}{k^2} (\kappa C \kappa)_{KM}^{-1} e^{i\mathbf{k} \cdot \mathbf{R}} d\mathbf{k}. \quad (\text{A.1})$$

For the calculation of Eq. (A.1), we use

$$d\mathbf{k} = k^2 \sin \theta dk d\theta d\phi \quad (\text{A.2})$$

with

$$\mathbf{k} \cdot \mathbf{R} = k \boldsymbol{\kappa} \cdot \mathbf{R}, \quad (\text{A.3})$$

where  $\boldsymbol{\kappa} = \mathbf{k}/k$  is a unit vector,  $k = |\mathbf{k}|$  and  $\boldsymbol{\kappa} = \boldsymbol{\kappa}(\theta, \phi)$ . Considering only the real part of the integral (A.1) since  $G_{KM}(\mathbf{R})$  is a real-valued tensor function, then Eq. (A.1) reads

$$G_{KM}(\mathbf{R}) = \frac{1}{(2\pi)^3} \int_0^{2\pi} \int_0^\pi \int_0^\infty (\kappa C \kappa)_{KM}^{-1} \cos(k \boldsymbol{\kappa} \cdot \mathbf{R}) dk \sin \theta d\theta d\phi. \quad (\text{A.4})$$

On the other hand, we can first perform the  $k$ -integration as follows [33]

$$\int_0^\infty \cos(k \boldsymbol{\kappa} \cdot \mathbf{R}) dk = \frac{1}{2} \int_{-\infty}^{+\infty} e^{ik \boldsymbol{\kappa} \cdot \mathbf{R}} dk = \pi \delta(\boldsymbol{\kappa} \cdot \mathbf{R}). \quad (\text{A.5})$$

Since

$$\boldsymbol{\kappa} \cdot \mathbf{R} = R \cos \theta, \quad (\text{A.6})$$

we obtain by means of the property of the  $\delta$ -function [33],  $\delta(ax) = \delta(x)/|a|$ ,

$$\delta(\boldsymbol{\kappa} \cdot \mathbf{R}) = \frac{1}{R} \delta(\cos \theta). \quad (\text{A.7})$$

In addition, we can write [52]

$$\delta(\cos \theta) = \delta(\theta - \pi/2), \quad 0 < \theta < \pi. \quad (\text{A.8})$$

After the  $\theta$ -integration, we find

$$G_{KM}(\mathbf{R}) = \frac{1}{8\pi^2 R} \int_0^{2\pi} (nCn)_{KM}^{-1} d\phi, \quad (\text{A.9})$$

where the integrand in Eq. (A.9) must be calculated for  $\theta = \pi/2$  and  $\boldsymbol{\kappa}$  becomes  $\mathbf{n} = \mathbf{n}(\phi) = \boldsymbol{\kappa}(\pi/2, \phi)$  with  $\mathbf{n} \cdot \mathbf{R} = 0$ . For arbitrary orthonormal vectors  $\mathbf{a}$  and  $\mathbf{b}$  in the plane  $\mathbf{n} \cdot \mathbf{R} = 0$ , the vector  $\mathbf{n}$  can be given by (see [6, 5])

$$\mathbf{n} = \mathbf{a} \cos \phi + \mathbf{b} \sin \phi. \quad (\text{A.10})$$

## B The first derivative of the Green tensor

In this Appendix, we calculate the first derivative of the Green tensor (29)

$$G_{IJ}(\mathbf{R}) = \frac{1}{8\pi^2 R} \int_0^{2\pi} (nCn)_{IJ}^{-1} d\phi. \quad (\text{B.1})$$

The differentiation of Eq. (B.1) with respect to  $x_k$  gives

$$G_{IJ,k}(\mathbf{R}) = \frac{1}{8\pi^2} \int_0^{2\pi} \left( (nCn)_{IJ}^{-1} \left( \frac{1}{R} \right)_{,k} + \frac{1}{R} (nCn)_{IJ,k}^{-1} \right) d\phi. \quad (\text{B.2})$$

Using the relations [16]

$$(nCn)_{IJ,k}^{-1} = -(nCn)_{IM}^{-1} (nCn)_{MN,k} (nCn)_{NJ}^{-1}, \quad (\text{B.3})$$

$$\left( \frac{1}{R} \right)_{,k} = -\frac{R_k}{R^3} = -\frac{\tau_k}{R^2}, \quad (\text{B.4})$$

$$(nCn)_{MN,k} = -\frac{n_k}{R} [(nC\tau)_{MN} + (\tau Cn)_{MN}], \quad (\text{B.5})$$

$$\delta n_k = -\frac{1}{R} n_j \delta x_j \tau_k, \quad (\text{B.6})$$

Eq. (B.2) becomes

$$G_{IJ,k}(\mathbf{R}) = -\frac{1}{8\pi^2 R^2} \int_0^{2\pi} \left( \tau_k (nCn)_{IJ}^{-1} - n_k (nCn)_{IM}^{-1} [(nC\tau)_{MN} + (\tau Cn)_{MN}] (nCn)_{NJ}^{-1} \right) d\phi, \quad (\text{B.7})$$

where  $\boldsymbol{\tau} = \mathbf{R}/R$ . Eq. (B.7) is analogous to the corresponding expression in anisotropic elasticity (see, e.g., [53, 16]).

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